



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:50 AM UTC

PDB ID : 6D1O / pdb_00006d1o
Title : FT_5 dioxygenase apoenzyme
Authors : Rydel, T.J.; Halls, C.E.
Deposited on : 2018-04-12
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

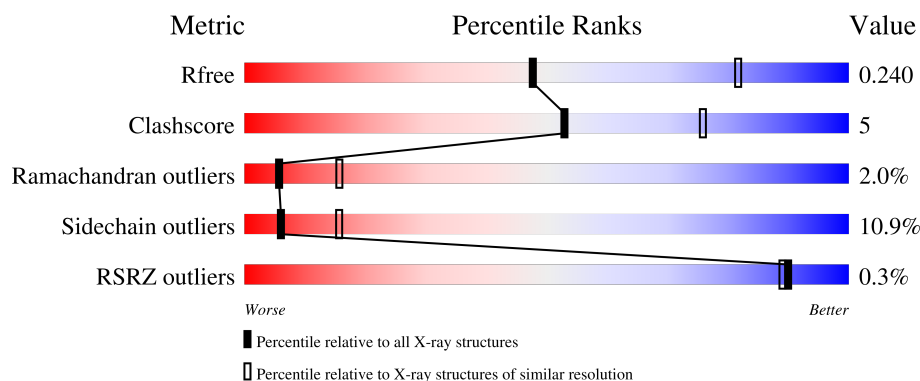
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	70% 15% .. 12%
1	B	301	69% 16% .. 13%
1	C	301	70% 16% .. 12%
1	D	301	% 67% 16% . . 12%
1	E	301	69% 13% . . 12%

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Mol	Chain	Length	Quality of chain
1	F	301	71%13%••13%
1	G	301	69%15%5%•9%
1	H	301	% 67%17%5%•8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17210 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2105	1343	358	395	9			
1	B	263	Total	C	N	O	S	0	0	0
			2094	1337	354	394	9			
1	C	266	Total	C	N	O	S	0	0	0
			2125	1354	364	398	9			
1	D	265	Total	C	N	O	S	0	0	0
			2117	1349	363	397	8			
1	E	266	Total	C	N	O	S	0	0	0
			2120	1352	363	397	8			
1	F	262	Total	C	N	O	S	0	0	0
			2092	1336	358	390	8			
1	G	275	Total	C	N	O	S	0	0	0
			2190	1391	379	412	8			
1	H	276	Total	C	N	O	S	0	0	0
			2194	1393	378	415	8			

There are 272 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	GLU	ASP	conflict	UNP Q8KSC8
A	109	ASN	ASP	conflict	UNP Q8KSC8
A	127	TYR	ARG	conflict	UNP Q8KSC8
A	129	LYS	ILE	conflict	UNP Q8KSC8
A	130	GLU	ASP	conflict	UNP Q8KSC8
A	131	ILE	VAL	conflict	UNP Q8KSC8
A	133	PRO	GLU	conflict	UNP Q8KSC8
A	134	TYR	HIS	conflict	UNP Q8KSC8
A	139	LEU	GLY	conflict	UNP Q8KSC8
A	141	THR	LEU	conflict	UNP Q8KSC8
A	209	GLU	GLY	conflict	UNP Q8KSC8
A	210	THR	SER	conflict	UNP Q8KSC8
A	229	SER	THR	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	230	GLU	ASP	conflict	UNP Q8KSC8
A	231	LYS	ALA	conflict	UNP Q8KSC8
A	234	GLU	LYS	conflict	UNP Q8KSC8
A	238	SER	GLN	conflict	UNP Q8KSC8
A	241	PHE	TYR	conflict	UNP Q8KSC8
A	242	ALA	GLU	conflict	UNP Q8KSC8
A	246	LYS	ARG	conflict	UNP Q8KSC8
A	247	PRO	PHE	conflict	UNP Q8KSC8
A	248	GLU	ASP	conflict	UNP Q8KSC8
A	256	GLN	LYS	conflict	UNP Q8KSC8
A	257	GLU	LYS	conflict	UNP Q8KSC8
A	258	GLY	ASP	conflict	UNP Q8KSC8
A	259	ASP	GLN	conflict	UNP Q8KSC8
A	269	GLN	MET	conflict	UNP Q8KSC8
A	271	TYR	ARG	conflict	UNP Q8KSC8
A	296	HIS	-	expression tag	UNP Q8KSC8
A	297	HIS	-	expression tag	UNP Q8KSC8
A	298	HIS	-	expression tag	UNP Q8KSC8
A	299	HIS	-	expression tag	UNP Q8KSC8
A	300	HIS	-	expression tag	UNP Q8KSC8
A	301	HIS	-	expression tag	UNP Q8KSC8
B	108	GLU	ASP	conflict	UNP Q8KSC8
B	109	ASN	ASP	conflict	UNP Q8KSC8
B	127	TYR	ARG	conflict	UNP Q8KSC8
B	129	LYS	ILE	conflict	UNP Q8KSC8
B	130	GLU	ASP	conflict	UNP Q8KSC8
B	131	ILE	VAL	conflict	UNP Q8KSC8
B	133	PRO	GLU	conflict	UNP Q8KSC8
B	134	TYR	HIS	conflict	UNP Q8KSC8
B	139	LEU	GLY	conflict	UNP Q8KSC8
B	141	THR	LEU	conflict	UNP Q8KSC8
B	209	GLU	GLY	conflict	UNP Q8KSC8
B	210	THR	SER	conflict	UNP Q8KSC8
B	229	SER	THR	conflict	UNP Q8KSC8
B	230	GLU	ASP	conflict	UNP Q8KSC8
B	231	LYS	ALA	conflict	UNP Q8KSC8
B	234	GLU	LYS	conflict	UNP Q8KSC8
B	238	SER	GLN	conflict	UNP Q8KSC8
B	241	PHE	TYR	conflict	UNP Q8KSC8
B	242	ALA	GLU	conflict	UNP Q8KSC8
B	246	LYS	ARG	conflict	UNP Q8KSC8
B	247	PRO	PHE	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	248	GLU	ASP	conflict	UNP Q8KSC8
B	256	GLN	LYS	conflict	UNP Q8KSC8
B	257	GLU	LYS	conflict	UNP Q8KSC8
B	258	GLY	ASP	conflict	UNP Q8KSC8
B	259	ASP	GLN	conflict	UNP Q8KSC8
B	269	GLN	MET	conflict	UNP Q8KSC8
B	271	TYR	ARG	conflict	UNP Q8KSC8
B	296	HIS	-	expression tag	UNP Q8KSC8
B	297	HIS	-	expression tag	UNP Q8KSC8
B	298	HIS	-	expression tag	UNP Q8KSC8
B	299	HIS	-	expression tag	UNP Q8KSC8
B	300	HIS	-	expression tag	UNP Q8KSC8
B	301	HIS	-	expression tag	UNP Q8KSC8
C	108	GLU	ASP	conflict	UNP Q8KSC8
C	109	ASN	ASP	conflict	UNP Q8KSC8
C	127	TYR	ARG	conflict	UNP Q8KSC8
C	129	LYS	ILE	conflict	UNP Q8KSC8
C	130	GLU	ASP	conflict	UNP Q8KSC8
C	131	ILE	VAL	conflict	UNP Q8KSC8
C	133	PRO	GLU	conflict	UNP Q8KSC8
C	134	TYR	HIS	conflict	UNP Q8KSC8
C	139	LEU	GLY	conflict	UNP Q8KSC8
C	141	THR	LEU	conflict	UNP Q8KSC8
C	209	GLU	GLY	conflict	UNP Q8KSC8
C	210	THR	SER	conflict	UNP Q8KSC8
C	229	SER	THR	conflict	UNP Q8KSC8
C	230	GLU	ASP	conflict	UNP Q8KSC8
C	231	LYS	ALA	conflict	UNP Q8KSC8
C	234	GLU	LYS	conflict	UNP Q8KSC8
C	238	SER	GLN	conflict	UNP Q8KSC8
C	241	PHE	TYR	conflict	UNP Q8KSC8
C	242	ALA	GLU	conflict	UNP Q8KSC8
C	246	LYS	ARG	conflict	UNP Q8KSC8
C	247	PRO	PHE	conflict	UNP Q8KSC8
C	248	GLU	ASP	conflict	UNP Q8KSC8
C	256	GLN	LYS	conflict	UNP Q8KSC8
C	257	GLU	LYS	conflict	UNP Q8KSC8
C	258	GLY	ASP	conflict	UNP Q8KSC8
C	259	ASP	GLN	conflict	UNP Q8KSC8
C	269	GLN	MET	conflict	UNP Q8KSC8
C	271	TYR	ARG	conflict	UNP Q8KSC8
C	296	HIS	-	expression tag	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	297	HIS	-	expression tag	UNP Q8KSC8
C	298	HIS	-	expression tag	UNP Q8KSC8
C	299	HIS	-	expression tag	UNP Q8KSC8
C	300	HIS	-	expression tag	UNP Q8KSC8
C	301	HIS	-	expression tag	UNP Q8KSC8
D	108	GLU	ASP	conflict	UNP Q8KSC8
D	109	ASN	ASP	conflict	UNP Q8KSC8
D	127	TYR	ARG	conflict	UNP Q8KSC8
D	129	LYS	ILE	conflict	UNP Q8KSC8
D	130	GLU	ASP	conflict	UNP Q8KSC8
D	131	ILE	VAL	conflict	UNP Q8KSC8
D	133	PRO	GLU	conflict	UNP Q8KSC8
D	134	TYR	HIS	conflict	UNP Q8KSC8
D	139	LEU	GLY	conflict	UNP Q8KSC8
D	141	THR	LEU	conflict	UNP Q8KSC8
D	209	GLU	GLY	conflict	UNP Q8KSC8
D	210	THR	SER	conflict	UNP Q8KSC8
D	229	SER	THR	conflict	UNP Q8KSC8
D	230	GLU	ASP	conflict	UNP Q8KSC8
D	231	LYS	ALA	conflict	UNP Q8KSC8
D	234	GLU	LYS	conflict	UNP Q8KSC8
D	238	SER	GLN	conflict	UNP Q8KSC8
D	241	PHE	TYR	conflict	UNP Q8KSC8
D	242	ALA	GLU	conflict	UNP Q8KSC8
D	246	LYS	ARG	conflict	UNP Q8KSC8
D	247	PRO	PHE	conflict	UNP Q8KSC8
D	248	GLU	ASP	conflict	UNP Q8KSC8
D	256	GLN	LYS	conflict	UNP Q8KSC8
D	257	GLU	LYS	conflict	UNP Q8KSC8
D	258	GLY	ASP	conflict	UNP Q8KSC8
D	259	ASP	GLN	conflict	UNP Q8KSC8
D	269	GLN	MET	conflict	UNP Q8KSC8
D	271	TYR	ARG	conflict	UNP Q8KSC8
D	296	HIS	-	expression tag	UNP Q8KSC8
D	297	HIS	-	expression tag	UNP Q8KSC8
D	298	HIS	-	expression tag	UNP Q8KSC8
D	299	HIS	-	expression tag	UNP Q8KSC8
D	300	HIS	-	expression tag	UNP Q8KSC8
D	301	HIS	-	expression tag	UNP Q8KSC8
E	108	GLU	ASP	conflict	UNP Q8KSC8
E	109	ASN	ASP	conflict	UNP Q8KSC8
E	127	TYR	ARG	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	129	LYS	ILE	conflict	UNP Q8KSC8
E	130	GLU	ASP	conflict	UNP Q8KSC8
E	131	ILE	VAL	conflict	UNP Q8KSC8
E	133	PRO	GLU	conflict	UNP Q8KSC8
E	134	TYR	HIS	conflict	UNP Q8KSC8
E	139	LEU	GLY	conflict	UNP Q8KSC8
E	141	THR	LEU	conflict	UNP Q8KSC8
E	209	GLU	GLY	conflict	UNP Q8KSC8
E	210	THR	SER	conflict	UNP Q8KSC8
E	229	SER	THR	conflict	UNP Q8KSC8
E	230	GLU	ASP	conflict	UNP Q8KSC8
E	231	LYS	ALA	conflict	UNP Q8KSC8
E	234	GLU	LYS	conflict	UNP Q8KSC8
E	238	SER	GLN	conflict	UNP Q8KSC8
E	241	PHE	TYR	conflict	UNP Q8KSC8
E	242	ALA	GLU	conflict	UNP Q8KSC8
E	246	LYS	ARG	conflict	UNP Q8KSC8
E	247	PRO	PHE	conflict	UNP Q8KSC8
E	248	GLU	ASP	conflict	UNP Q8KSC8
E	256	GLN	LYS	conflict	UNP Q8KSC8
E	257	GLU	LYS	conflict	UNP Q8KSC8
E	258	GLY	ASP	conflict	UNP Q8KSC8
E	259	ASP	GLN	conflict	UNP Q8KSC8
E	269	GLN	MET	conflict	UNP Q8KSC8
E	271	TYR	ARG	conflict	UNP Q8KSC8
E	296	HIS	-	expression tag	UNP Q8KSC8
E	297	HIS	-	expression tag	UNP Q8KSC8
E	298	HIS	-	expression tag	UNP Q8KSC8
E	299	HIS	-	expression tag	UNP Q8KSC8
E	300	HIS	-	expression tag	UNP Q8KSC8
E	301	HIS	-	expression tag	UNP Q8KSC8
F	108	GLU	ASP	conflict	UNP Q8KSC8
F	109	ASN	ASP	conflict	UNP Q8KSC8
F	127	TYR	ARG	conflict	UNP Q8KSC8
F	129	LYS	ILE	conflict	UNP Q8KSC8
F	130	GLU	ASP	conflict	UNP Q8KSC8
F	131	ILE	VAL	conflict	UNP Q8KSC8
F	133	PRO	GLU	conflict	UNP Q8KSC8
F	134	TYR	HIS	conflict	UNP Q8KSC8
F	139	LEU	GLY	conflict	UNP Q8KSC8
F	141	THR	LEU	conflict	UNP Q8KSC8
F	209	GLU	GLY	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	210	THR	SER	conflict	UNP Q8KSC8
F	229	SER	THR	conflict	UNP Q8KSC8
F	230	GLU	ASP	conflict	UNP Q8KSC8
F	231	LYS	ALA	conflict	UNP Q8KSC8
F	234	GLU	LYS	conflict	UNP Q8KSC8
F	238	SER	GLN	conflict	UNP Q8KSC8
F	241	PHE	TYR	conflict	UNP Q8KSC8
F	242	ALA	GLU	conflict	UNP Q8KSC8
F	246	LYS	ARG	conflict	UNP Q8KSC8
F	247	PRO	PHE	conflict	UNP Q8KSC8
F	248	GLU	ASP	conflict	UNP Q8KSC8
F	256	GLN	LYS	conflict	UNP Q8KSC8
F	257	GLU	LYS	conflict	UNP Q8KSC8
F	258	GLY	ASP	conflict	UNP Q8KSC8
F	259	ASP	GLN	conflict	UNP Q8KSC8
F	269	GLN	MET	conflict	UNP Q8KSC8
F	271	TYR	ARG	conflict	UNP Q8KSC8
F	296	HIS	-	expression tag	UNP Q8KSC8
F	297	HIS	-	expression tag	UNP Q8KSC8
F	298	HIS	-	expression tag	UNP Q8KSC8
F	299	HIS	-	expression tag	UNP Q8KSC8
F	300	HIS	-	expression tag	UNP Q8KSC8
F	301	HIS	-	expression tag	UNP Q8KSC8
G	108	GLU	ASP	conflict	UNP Q8KSC8
G	109	ASN	ASP	conflict	UNP Q8KSC8
G	127	TYR	ARG	conflict	UNP Q8KSC8
G	129	LYS	ILE	conflict	UNP Q8KSC8
G	130	GLU	ASP	conflict	UNP Q8KSC8
G	131	ILE	VAL	conflict	UNP Q8KSC8
G	133	PRO	GLU	conflict	UNP Q8KSC8
G	134	TYR	HIS	conflict	UNP Q8KSC8
G	139	LEU	GLY	conflict	UNP Q8KSC8
G	141	THR	LEU	conflict	UNP Q8KSC8
G	209	GLU	GLY	conflict	UNP Q8KSC8
G	210	THR	SER	conflict	UNP Q8KSC8
G	229	SER	THR	conflict	UNP Q8KSC8
G	230	GLU	ASP	conflict	UNP Q8KSC8
G	231	LYS	ALA	conflict	UNP Q8KSC8
G	234	GLU	LYS	conflict	UNP Q8KSC8
G	238	SER	GLN	conflict	UNP Q8KSC8
G	241	PHE	TYR	conflict	UNP Q8KSC8
G	242	ALA	GLU	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	246	LYS	ARG	conflict	UNP Q8KSC8
G	247	PRO	PHE	conflict	UNP Q8KSC8
G	248	GLU	ASP	conflict	UNP Q8KSC8
G	256	GLN	LYS	conflict	UNP Q8KSC8
G	257	GLU	LYS	conflict	UNP Q8KSC8
G	258	GLY	ASP	conflict	UNP Q8KSC8
G	259	ASP	GLN	conflict	UNP Q8KSC8
G	269	GLN	MET	conflict	UNP Q8KSC8
G	271	TYR	ARG	conflict	UNP Q8KSC8
G	296	HIS	-	expression tag	UNP Q8KSC8
G	297	HIS	-	expression tag	UNP Q8KSC8
G	298	HIS	-	expression tag	UNP Q8KSC8
G	299	HIS	-	expression tag	UNP Q8KSC8
G	300	HIS	-	expression tag	UNP Q8KSC8
G	301	HIS	-	expression tag	UNP Q8KSC8
H	108	GLU	ASP	conflict	UNP Q8KSC8
H	109	ASN	ASP	conflict	UNP Q8KSC8
H	127	TYR	ARG	conflict	UNP Q8KSC8
H	129	LYS	ILE	conflict	UNP Q8KSC8
H	130	GLU	ASP	conflict	UNP Q8KSC8
H	131	ILE	VAL	conflict	UNP Q8KSC8
H	133	PRO	GLU	conflict	UNP Q8KSC8
H	134	TYR	HIS	conflict	UNP Q8KSC8
H	139	LEU	GLY	conflict	UNP Q8KSC8
H	141	THR	LEU	conflict	UNP Q8KSC8
H	209	GLU	GLY	conflict	UNP Q8KSC8
H	210	THR	SER	conflict	UNP Q8KSC8
H	229	SER	THR	conflict	UNP Q8KSC8
H	230	GLU	ASP	conflict	UNP Q8KSC8
H	231	LYS	ALA	conflict	UNP Q8KSC8
H	234	GLU	LYS	conflict	UNP Q8KSC8
H	238	SER	GLN	conflict	UNP Q8KSC8
H	241	PHE	TYR	conflict	UNP Q8KSC8
H	242	ALA	GLU	conflict	UNP Q8KSC8
H	246	LYS	ARG	conflict	UNP Q8KSC8
H	247	PRO	PHE	conflict	UNP Q8KSC8
H	248	GLU	ASP	conflict	UNP Q8KSC8
H	256	GLN	LYS	conflict	UNP Q8KSC8
H	257	GLU	LYS	conflict	UNP Q8KSC8
H	258	GLY	ASP	conflict	UNP Q8KSC8
H	259	ASP	GLN	conflict	UNP Q8KSC8
H	269	GLN	MET	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	271	TYR	ARG	conflict	UNP Q8KSC8
H	296	HIS	-	expression tag	UNP Q8KSC8
H	297	HIS	-	expression tag	UNP Q8KSC8
H	298	HIS	-	expression tag	UNP Q8KSC8
H	299	HIS	-	expression tag	UNP Q8KSC8
H	300	HIS	-	expression tag	UNP Q8KSC8
H	301	HIS	-	expression tag	UNP Q8KSC8

- Molecule 2 is water.

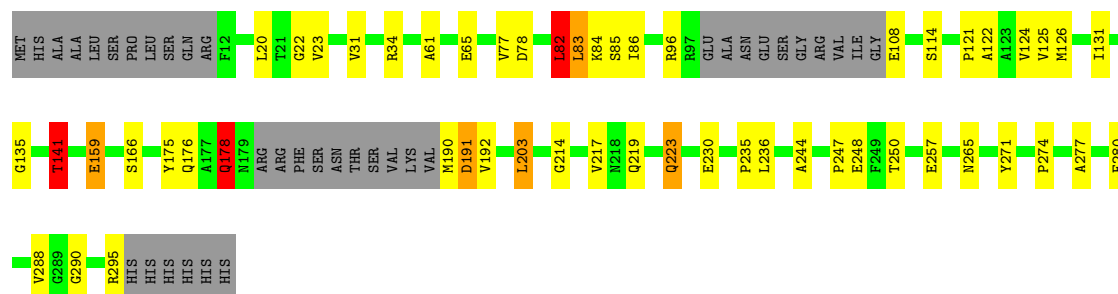
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	19	Total O 19 19	0	0
2	B	23	Total O 23 23	0	0
2	C	17	Total O 17 17	0	0
2	D	14	Total O 14 14	0	0
2	E	35	Total O 35 35	0	0
2	F	34	Total O 34 34	0	0
2	G	17	Total O 17 17	0	0
2	H	14	Total O 14 14	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

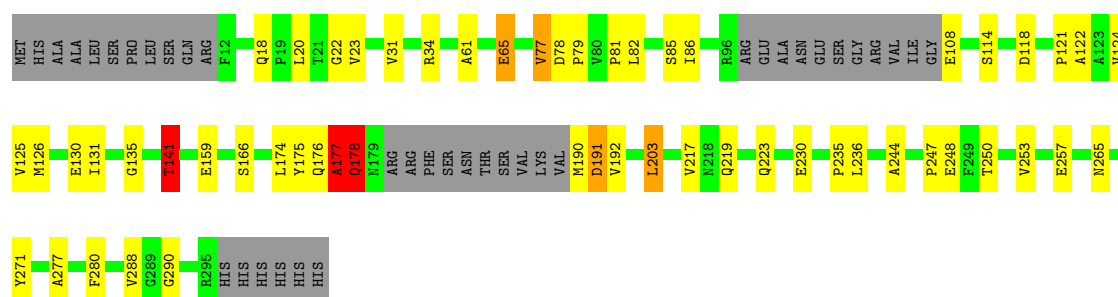
- Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

Chain A: 



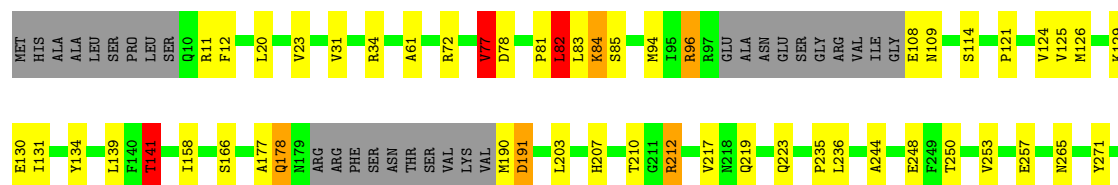
- Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

Chain B: 



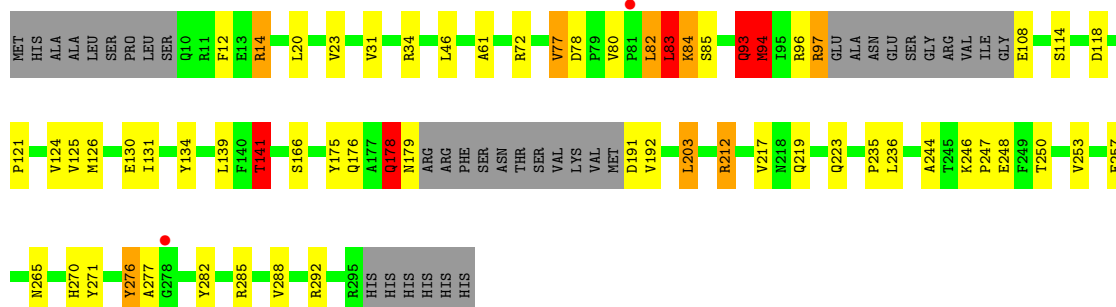
- Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

Chain C: 

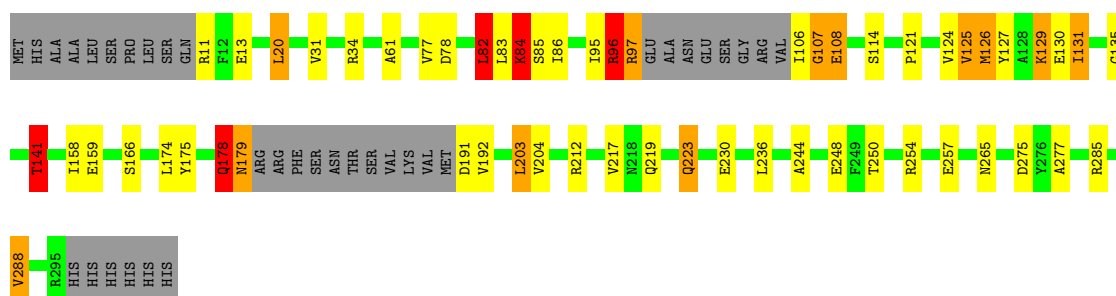




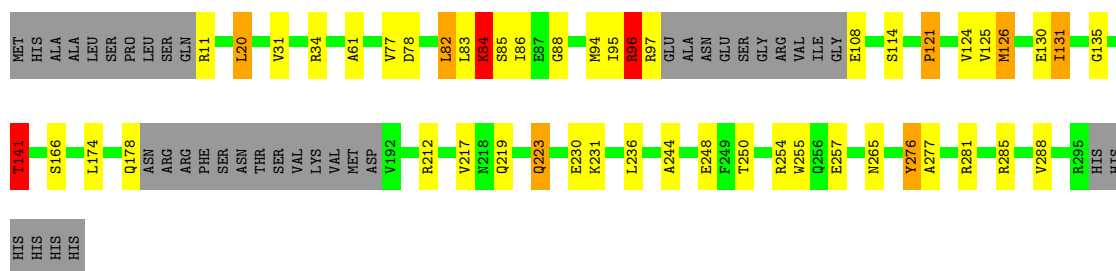
- Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase



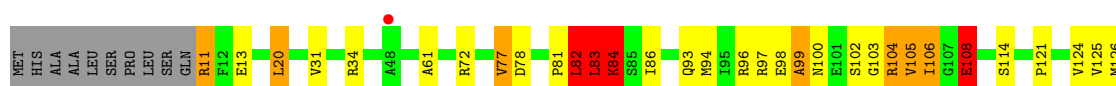
- Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

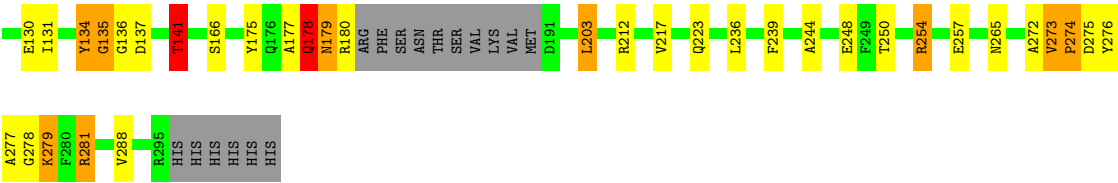


- Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

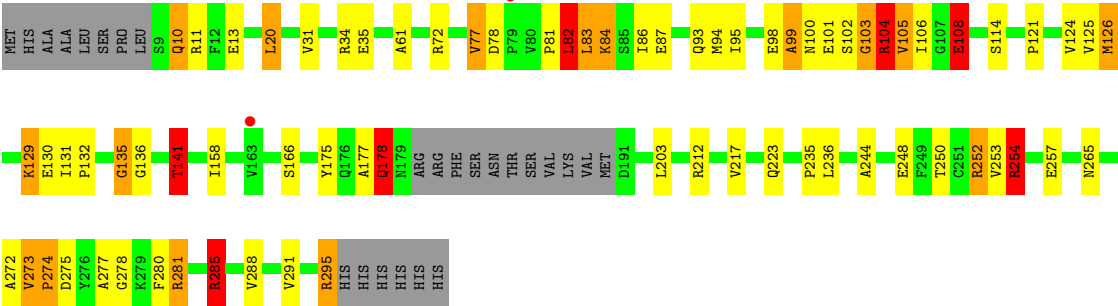


- Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase





• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.46Å 200.33Å 98.31Å 90.00° 110.95° 90.00°	Depositor
Resolution (Å)	46.19 – 2.70 46.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (46.19-2.70) 97.3 (46.19-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.213 , 0.241 0.213 , 0.240	Depositor DCC
R_{free} test set	3513 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	1.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.460 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17210	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.26	5/2162 (0.2%)	1.26	10/2949 (0.3%)
1	B	1.29	7/2151 (0.3%)	1.25	9/2935 (0.3%)
1	C	1.12	3/2182 (0.1%)	1.23	12/2975 (0.4%)
1	D	1.15	4/2174 (0.2%)	1.28	19/2965 (0.6%)
1	E	1.32	10/2177 (0.5%)	1.31	18/2969 (0.6%)
1	F	1.27	4/2149 (0.2%)	1.26	10/2931 (0.3%)
1	G	1.26	9/2248 (0.4%)	1.36	21/3065 (0.7%)
1	H	1.26	14/2252 (0.6%)	1.34	20/3071 (0.7%)
All	All	1.24	56/17495 (0.3%)	1.29	119/23860 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	E	0	1
1	F	0	1
1	G	0	2
1	H	0	2
All	All	0	8

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	ASP	CB-CG	8.27	1.72	1.52
1	B	81	PRO	C-O	8.23	1.34	1.24
1	B	78	ASP	CB-CG	8.13	1.72	1.52
1	E	78	ASP	N-CA	-7.36	1.36	1.45
1	F	78	ASP	N-CA	-7.33	1.36	1.45
1	B	159	GLU	CD-OE2	7.16	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	273	VAL	C-O	-7.00	1.15	1.24
1	H	99	ALA	CA-C	-6.98	1.44	1.52
1	E	275	ASP	C-O	-6.92	1.16	1.24
1	G	83	LEU	C-O	-6.53	1.15	1.24
1	D	14	ARG	CB-CG	-6.52	1.32	1.52
1	E	223	GLN	CA-C	6.48	1.58	1.52
1	H	178	GLN	CA-C	6.47	1.61	1.52
1	H	98	GLU	CA-C	-6.37	1.47	1.53
1	G	274	PRO	N-CA	-6.31	1.39	1.47
1	G	78	ASP	CB-CG	6.27	1.67	1.52
1	A	159	GLU	CG-CD	6.17	1.67	1.52
1	H	273	VAL	C-O	-6.09	1.16	1.24
1	E	159	GLU	CD-OE1	6.07	1.36	1.25
1	E	96	ARG	CA-C	6.01	1.60	1.52
1	E	159	GLU	CD-OE2	5.86	1.36	1.25
1	B	178	GLN	CA-CB	5.83	1.63	1.53
1	H	78	ASP	CB-CG	5.82	1.66	1.52
1	D	219	GLN	CD-OE1	5.81	1.34	1.23
1	H	178	GLN	N-CA	5.77	1.53	1.46
1	F	223	GLN	CA-C	5.74	1.58	1.52
1	H	84	LYS	CA-C	5.69	1.60	1.52
1	H	274	PRO	N-CA	-5.67	1.40	1.47
1	C	253	VAL	N-CA	-5.61	1.39	1.46
1	H	135	GLY	C-O	-5.60	1.16	1.23
1	G	135	GLY	C-O	-5.56	1.16	1.23
1	H	277	ALA	CA-CB	-5.53	1.45	1.53
1	G	141	THR	CA-C	-5.52	1.46	1.52
1	H	141	THR	CA-C	-5.43	1.46	1.52
1	C	177	ALA	C-O	-5.43	1.17	1.24
1	G	99	ALA	CA-C	-5.38	1.45	1.52
1	D	178	GLN	N-CA	5.35	1.53	1.46
1	D	253	VAL	N-CA	-5.34	1.39	1.46
1	A	65	GLU	CG-CD	5.33	1.65	1.52
1	G	98	GLU	CA-C	-5.31	1.46	1.52
1	B	79	PRO	C-O	-5.29	1.17	1.23
1	H	10	GLN	N-CA	5.27	1.52	1.46
1	A	223	GLN	CA-C	5.25	1.57	1.52
1	B	253	VAL	N-CA	-5.21	1.39	1.46
1	E	158	ILE	C-O	-5.20	1.19	1.24
1	F	141	THR	CA-C	-5.20	1.46	1.52
1	E	219	GLN	CD-OE1	5.19	1.33	1.23
1	G	134	TYR	C-O	-5.18	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	141	THR	CA-C	-5.17	1.46	1.52
1	A	214	GLY	CA-C	5.14	1.56	1.52
1	C	219	GLN	CD-OE1	5.13	1.33	1.23
1	H	253	VAL	N-CA	-5.11	1.39	1.46
1	B	65	GLU	CG-CD	5.10	1.64	1.52
1	F	121	PRO	N-CA	-5.10	1.40	1.47
1	E	13	GLU	CD-OE2	5.09	1.35	1.25
1	H	291	VAL	CA-C	-5.07	1.46	1.52

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	ARG	CG-CD-NE	-11.86	85.91	112.00
1	B	177	ALA	CA-C-O	-10.91	104.91	120.51
1	D	82	LEU	CA-CB-CG	9.64	150.05	116.30
1	F	82	LEU	CA-CB-CG	9.64	150.05	116.30
1	A	159	GLU	CB-CG-CD	9.61	128.94	112.60
1	H	82	LEU	CA-CB-CG	9.28	148.79	116.30
1	H	277	ALA	N-CA-C	-8.81	94.83	109.46
1	G	277	ALA	N-CA-C	-8.64	95.12	109.46
1	C	12	PHE	N-CA-C	-8.53	94.35	108.34
1	H	252	ARG	CG-CD-NE	8.38	130.42	112.00
1	E	96	ARG	N-CA-CB	-8.35	97.37	111.31
1	E	82	LEU	CA-CB-CG	8.33	145.44	116.30
1	D	12	PHE	N-CA-C	-8.12	95.02	108.34
1	G	179	ASN	N-CA-C	8.10	128.06	110.80
1	G	281	ARG	CA-CB-CG	7.93	129.96	114.10
1	E	129	LYS	CB-CG-CD	7.74	129.10	111.30
1	D	14	ARG	CB-CG-CD	7.58	128.72	111.30
1	H	281	ARG	CA-CB-CG	7.52	129.13	114.10
1	D	12	PHE	N-CA-CB	-7.42	99.12	110.77
1	C	12	PHE	N-CA-CB	-7.29	99.32	110.77
1	G	108	GLU	CB-CG-CD	7.26	124.94	112.60
1	C	96	ARG	N-CA-C	7.22	118.12	108.38
1	G	279	LYS	CB-CG-CD	7.16	127.77	111.30
1	A	82	LEU	CB-CG-CD2	7.12	132.05	110.70
1	G	136	GLY	N-CA-C	-6.94	96.73	113.18
1	D	94	MET	CA-CB-CG	6.88	127.86	114.10
1	H	136	GLY	N-CA-C	-6.87	96.89	113.18
1	H	108	GLU	CB-CG-CD	6.82	124.19	112.60
1	F	96	ARG	CB-CG-CD	6.77	126.86	111.30
1	G	82	LEU	CA-CB-CG	6.73	139.86	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	LYS	CB-CG-CD	6.71	126.74	111.30
1	D	97	ARG	CA-CB-CG	6.67	127.44	114.10
1	G	178	GLN	N-CA-C	6.59	124.85	110.80
1	H	275	ASP	N-CA-CB	-6.54	98.39	110.56
1	A	295	ARG	CG-CD-NE	-6.36	98.00	112.00
1	G	274	PRO	CB-CA-C	-6.33	103.14	111.23
1	H	106	ILE	N-CA-C	6.32	122.49	109.34
1	B	219	GLN	N-CA-CB	-6.28	99.97	110.39
1	G	275	ASP	N-CA-CB	-6.26	98.92	110.56
1	A	219	GLN	N-CA-CB	-6.23	100.05	110.39
1	H	285	ARG	CA-CB-CG	6.17	126.43	114.10
1	E	114	SER	N-CA-C	6.15	119.88	111.39
1	H	274	PRO	CB-CA-C	-6.14	103.37	111.23
1	E	107	GLY	N-CA-C	6.12	127.69	113.18
1	C	82	LEU	N-CA-CB	6.10	120.81	110.49
1	G	106	ILE	N-CA-C	6.09	122.00	109.34
1	H	141	THR	CB-CA-C	-6.06	97.91	109.66
1	H	84	LYS	CA-C-O	6.00	129.08	120.51
1	H	295	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	159	GLU	CG-CD-OE1	5.98	132.16	118.40
1	C	82	LEU	CA-CB-CG	5.97	137.20	116.30
1	G	141	THR	CB-CA-C	-5.97	98.08	109.66
1	D	23	VAL	CB-CA-C	-5.91	105.63	111.30
1	E	219	GLN	N-CA-CB	-5.85	100.68	110.39
1	C	141	THR	CB-CA-C	-5.85	98.31	109.66
1	F	114	SER	N-CA-C	5.84	119.46	111.39
1	D	141	THR	CB-CA-C	-5.84	98.33	109.66
1	D	178	GLN	N-CA-C	5.84	123.24	110.80
1	E	141	THR	CB-CA-C	-5.77	98.47	109.66
1	G	275	ASP	N-CA-C	5.76	119.05	107.41
1	C	23	VAL	CB-CA-C	-5.75	105.78	111.30
1	E	96	ARG	CA-CB-CG	5.74	125.59	114.10
1	C	191	ASP	N-CA-CB	5.74	118.30	109.98
1	F	131	ILE	CB-CG1-CD1	5.72	125.82	113.80
1	F	141	THR	CB-CA-C	-5.72	98.55	109.66
1	H	178	GLN	N-CA-C	5.72	122.98	110.80
1	H	275	ASP	N-CA-C	5.71	118.94	107.41
1	A	192	VAL	N-CA-C	5.70	115.90	110.42
1	D	118	ASP	OD1-CG-OD2	-5.70	109.23	122.90
1	H	295	ARG	NH1-CZ-NH2	-5.67	111.92	119.30
1	B	141	THR	CB-CA-C	-5.66	98.68	109.66
1	H	103	GLY	N-CA-C	5.66	126.58	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	THR	CB-CA-C	-5.63	98.73	109.66
1	D	93	GLN	CB-CG-CD	-5.63	103.03	112.60
1	E	159	GLU	CA-CB-CG	5.62	125.33	114.10
1	C	219	GLN	N-CA-CB	-5.60	101.09	110.39
1	D	176	GLN	CA-CB-CG	5.60	125.30	114.10
1	D	83	LEU	N-CA-CB	-5.57	102.17	111.20
1	F	219	GLN	N-CA-CB	-5.53	101.21	110.39
1	D	114	SER	N-CA-C	5.50	118.98	111.39
1	G	82	LEU	CB-CG-CD1	5.49	127.16	110.70
1	G	82	LEU	N-CA-CB	5.48	119.75	110.49
1	A	191	ASP	N-CA-CB	5.47	117.92	109.98
1	D	219	GLN	N-CA-CB	-5.46	101.33	110.39
1	C	83	LEU	CA-C-N	5.45	128.37	120.79
1	C	83	LEU	C-N-CA	5.45	128.37	120.79
1	G	277	ALA	CA-C-O	-5.41	114.42	120.54
1	B	191	ASP	N-CA-CB	5.40	117.82	109.98
1	G	114	SER	N-CA-C	5.40	118.84	111.39
1	E	131	ILE	CB-CG1-CD1	5.40	125.13	113.80
1	B	82	LEU	CA-CB-CG	5.34	135.01	116.30
1	C	114	SER	N-CA-C	5.34	118.76	111.39
1	B	192	VAL	N-CA-C	5.29	115.50	110.42
1	H	130	GLU	CB-CG-CD	5.26	121.53	112.60
1	F	97	ARG	N-CA-CB	5.25	119.43	110.50
1	H	114	SER	N-CA-C	5.23	118.61	111.39
1	B	23	VAL	CB-CA-C	-5.21	106.30	111.30
1	A	23	VAL	CB-CA-C	-5.20	106.30	111.30
1	F	84	LYS	N-CA-C	5.20	121.88	110.80
1	F	11	ARG	CA-C-O	5.20	129.63	120.80
1	G	96	ARG	CA-CB-CG	5.19	124.48	114.10
1	G	130	GLU	CB-CG-CD	5.19	121.42	112.60
1	E	192	VAL	N-CA-C	5.19	115.40	110.42
1	F	11	ARG	CB-CA-C	5.17	119.92	110.10
1	E	78	ASP	CA-CB-CG	-5.15	107.45	112.60
1	E	125	VAL	CB-CA-C	5.09	118.00	110.77
1	B	114	SER	N-CA-C	5.09	118.42	111.39
1	E	204	VAL	CB-CA-C	-5.08	102.92	110.33
1	A	114	SER	N-CA-C	5.07	118.39	111.39
1	E	288	VAL	CA-C-N	5.06	126.25	120.53
1	E	288	VAL	C-N-CA	5.06	126.25	120.53
1	B	178	GLN	CA-CB-CG	5.05	124.20	114.10
1	E	108	GLU	N-CA-C	5.05	116.66	109.14
1	E	84	LYS	N-CA-C	5.05	121.55	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	137	ASP	CB-CG-OD2	-5.04	106.80	118.40
1	D	192	VAL	N-CA-C	5.03	115.25	110.42
1	H	254	ARG	CB-CG-CD	5.03	122.86	111.30
1	G	137	ASP	N-CA-CB	5.02	118.78	110.69
1	D	179	ASN	N-CA-C	5.02	125.06	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	77	VAL	Peptide
1	C	77	VAL	Peptide
1	E	107	GLY	Peptide
1	F	96	ARG	Peptide
1	G	81	PRO	Peptide
1	G	82	LEU	Peptide
1	H	104	ARG	Peptide
1	H	82	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2105	0	2030	16	0
1	B	2094	0	2017	17	0
1	C	2125	0	2051	22	0
1	D	2117	0	2042	31	0
1	E	2120	0	2048	23	0
1	F	2092	0	2024	19	0
1	G	2190	0	2115	31	0
1	H	2194	0	2115	43	0
2	A	19	0	0	1	0
2	B	23	0	0	1	0
2	C	17	0	0	1	0
2	D	14	0	0	1	0
2	E	35	0	0	1	0
2	F	34	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	17	0	0	3	0
2	H	14	0	0	2	0
All	All	17210	0	16442	167	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LEU:HD23	1:H:101:GLU:HG3	1.20	1.14
1:D:212:ARG:HG2	1:H:280:PHE:CD2	1.95	1.02
1:D:80:VAL:O	1:D:83:LEU:HB3	1.66	0.93
1:G:99:ALA:HB2	1:G:278:GLY:HA3	1.50	0.91
1:A:274:PRO:HB2	1:H:87:GLU:OE2	1.72	0.90
1:C:108:GLU:HG3	1:C:109:ASN:N	1.92	0.83
1:E:178:GLN:O	1:E:178:GLN:NE2	2.13	0.80
1:D:212:ARG:HG2	1:H:280:PHE:CG	2.17	0.79
1:G:83:LEU:HB3	1:G:84:LYS:HE3	1.63	0.79
1:G:82:LEU:O	1:G:83:LEU:HB2	1.84	0.75
1:C:210:THR:HG23	1:C:212:ARG:H	1.52	0.75
1:G:83:LEU:HB3	1:G:84:LYS:CE	2.17	0.73
1:E:174:LEU:HD23	1:G:177:ALA:HB1	1.71	0.73
1:C:207:HIS:HB3	1:C:210:THR:HG22	1.71	0.72
1:A:141:THR:HG23	1:A:250:THR:HG22	1.72	0.72
1:C:141:THR:HG23	1:C:250:THR:HG22	1.72	0.71
1:B:141:THR:HG23	1:B:250:THR:HG22	1.72	0.71
1:F:82:LEU:O	1:F:83:LEU:HD23	1.91	0.71
1:F:141:THR:HG23	1:F:250:THR:HG22	1.72	0.70
1:H:99:ALA:HB2	1:H:278:GLY:HA3	1.73	0.70
1:D:141:THR:HG23	1:D:250:THR:HG22	1.72	0.70
1:E:82:LEU:O	1:E:83:LEU:HD23	1.91	0.70
1:D:212:ARG:CG	1:H:280:PHE:CG	2.75	0.69
1:G:141:THR:HG23	1:G:250:THR:HG22	1.74	0.69
1:H:141:THR:HG23	1:H:250:THR:HG22	1.74	0.69
1:E:141:THR:HG23	1:E:250:THR:HG22	1.74	0.69
1:F:174:LEU:HD23	1:H:177:ALA:HB1	1.75	0.68
1:H:81:PRO:O	1:H:82:LEU:HD22	1.97	0.65
1:A:82:LEU:O	1:A:83:LEU:HD12	1.96	0.64
1:C:158:ILE:HB	1:C:203:LEU:CD2	2.28	0.64
1:C:84:LYS:HG3	1:C:94:MET:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LEU:CD2	1:H:101:GLU:HG3	2.12	0.63
1:B:65:GLU:HB2	2:B:404:HOH:O	1.98	0.62
1:B:176:GLN:O	1:B:177:ALA:O	2.17	0.62
1:H:100:ASN:ND2	1:H:104:ARG:O	2.33	0.62
1:F:126:MET:HE3	1:F:285:ARG:HB2	1.81	0.62
1:C:131:ILE:HD11	2:C:408:HOH:O	2.00	0.62
1:E:126:MET:HE3	1:E:285:ARG:HB2	1.82	0.61
1:B:174:LEU:O	1:B:178:GLN:NE2	2.34	0.61
1:F:131:ILE:HG13	1:F:257:GLU:HG3	1.83	0.59
1:H:99:ALA:HB2	1:H:278:GLY:CA	2.31	0.59
1:G:99:ALA:HB2	1:G:278:GLY:CA	2.30	0.59
1:B:203:LEU:O	1:B:203:LEU:HD12	2.03	0.59
1:C:81:PRO:O	1:C:82:LEU:HD22	2.02	0.59
1:E:11:ARG:N	2:E:401:HOH:O	2.35	0.59
1:A:175:TYR:O	1:A:178:GLN:HG3	2.03	0.58
1:A:203:LEU:HD12	1:A:203:LEU:O	2.03	0.58
1:C:235:PRO:HB2	1:D:235:PRO:HB2	1.85	0.58
1:D:203:LEU:HD12	1:D:203:LEU:O	2.03	0.58
1:E:175:TYR:O	1:E:178:GLN:HG3	2.04	0.58
1:G:203:LEU:HD12	1:G:203:LEU:O	2.04	0.58
1:D:80:VAL:O	1:D:83:LEU:CB	2.47	0.57
1:B:175:TYR:O	1:B:178:GLN:HG2	2.04	0.57
1:E:131:ILE:HG13	1:E:257:GLU:HG3	1.86	0.57
1:D:175:TYR:O	1:D:178:GLN:HG3	2.04	0.57
1:D:212:ARG:HD3	1:H:280:PHE:CZ	2.39	0.57
1:E:203:LEU:HD12	1:E:203:LEU:O	2.04	0.56
1:E:174:LEU:HD23	1:G:177:ALA:CB	2.35	0.56
1:E:127:TYR:CD2	1:E:129:LYS:HD3	2.42	0.54
1:G:175:TYR:O	1:G:178:GLN:HG2	2.07	0.54
1:C:84:LYS:HG3	1:C:94:MET:CG	2.38	0.54
1:E:248:GLU:HA	1:H:273:VAL:CG1	2.37	0.54
1:G:108:GLU:HG3	1:G:272:ALA:O	2.08	0.54
1:H:175:TYR:O	1:H:178:GLN:HG2	2.07	0.54
1:C:207:HIS:CB	1:C:210:THR:HG22	2.38	0.53
1:F:84:LYS:HG3	1:F:94:MET:O	2.08	0.53
1:H:131:ILE:HD12	1:H:132:PRO:O	2.08	0.53
1:B:248:GLU:OE1	1:C:271:TYR:OH	2.22	0.53
1:D:94:MET:HG3	1:D:282:TYR:HE1	1.74	0.52
1:D:97:ARG:NH2	1:D:276:TYR:OH	2.41	0.52
1:F:174:LEU:HD23	1:H:177:ALA:CB	2.39	0.52
1:D:131:ILE:HG13	1:D:257:GLU:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLY:HA2	1:C:134:TYR:CE1	2.45	0.51
1:D:46:LEU:HD23	1:H:101:GLU:CG	2.13	0.51
1:H:94:MET:C	1:H:95:ILE:HD12	2.35	0.51
1:H:158:ILE:HB	1:H:203:LEU:CD2	2.40	0.51
1:A:248:GLU:OE1	1:D:271:TYR:OH	2.25	0.51
1:E:34:ARG:HD3	1:E:61:ALA:O	2.11	0.51
1:F:248:GLU:HA	1:G:273:VAL:CG1	2.40	0.51
1:D:72:ARG:HG2	1:D:77:VAL:HG13	1.93	0.51
1:F:34:ARG:HD3	1:F:61:ALA:O	2.11	0.51
1:G:11:ARG:N	2:G:402:HOH:O	2.43	0.51
1:F:88:GLY:HA2	2:F:406:HOH:O	2.11	0.51
1:B:131:ILE:HG13	1:B:257:GLU:HG3	1.93	0.51
1:F:255:TRP:CD1	1:F:281:ARG:NH2	2.79	0.51
1:H:108:GLU:HG3	1:H:272:ALA:O	2.11	0.50
1:G:131:ILE:HG13	1:G:257:GLU:HG3	1.92	0.50
1:A:131:ILE:HG13	1:A:257:GLU:HG3	1.92	0.50
1:C:131:ILE:HG13	1:C:257:GLU:HG3	1.92	0.50
1:E:106:ILE:HG23	1:H:248:GLU:OE2	2.11	0.50
1:F:141:THR:HG21	1:F:244:ALA:O	2.12	0.49
1:C:72:ARG:HG2	1:C:77:VAL:HG13	1.94	0.49
1:B:34:ARG:HD3	1:B:61:ALA:O	2.12	0.49
1:C:207:HIS:HB3	1:C:210:THR:CG2	2.41	0.49
1:E:141:THR:HG21	1:E:244:ALA:O	2.13	0.49
1:G:83:LEU:HB3	1:G:84:LYS:HE2	1.95	0.49
1:D:34:ARG:HD3	1:D:61:ALA:O	2.13	0.49
1:D:212:ARG:HG3	1:H:280:PHE:CG	2.48	0.49
1:C:34:ARG:HD3	1:C:61:ALA:O	2.13	0.48
1:A:34:ARG:HD3	1:A:61:ALA:O	2.13	0.48
1:B:122:ALA:HB2	1:B:290:GLY:HA3	1.96	0.48
1:G:105:VAL:CG1	1:G:274:PRO:HB3	2.43	0.48
1:H:252:ARG:NH1	2:H:402:HOH:O	2.46	0.48
1:A:271:TYR:OH	1:D:248:GLU:OE1	2.28	0.48
1:F:254:ARG:HH12	1:G:20:LEU:HA	1.78	0.48
1:E:96:ARG:CG	1:E:96:ARG:HH11	2.26	0.47
1:A:22:GLY:HA2	1:D:134:TYR:CE1	2.49	0.47
1:C:141:THR:HG21	1:C:244:ALA:O	2.15	0.47
1:H:141:THR:HG21	1:H:244:ALA:O	2.15	0.47
1:H:93:GLN:HB2	1:H:285:ARG:HG2	1.96	0.47
1:G:141:THR:HG21	1:G:244:ALA:O	2.15	0.47
1:G:105:VAL:HG11	1:G:274:PRO:HB3	1.97	0.47
1:G:72:ARG:HG2	1:G:77:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLN:C	1:B:177:ALA:O	2.59	0.46
1:D:141:THR:HG21	1:D:244:ALA:O	2.16	0.46
1:A:247:PRO:HB3	1:D:139:LEU:HD11	1.98	0.46
1:G:93:GLN:HG3	2:G:401:HOH:O	2.16	0.46
1:F:88:GLY:CA	2:F:406:HOH:O	2.63	0.46
1:D:212:ARG:CG	1:H:280:PHE:CD2	2.84	0.45
1:A:122:ALA:HB2	1:A:290:GLY:HA3	1.97	0.45
1:A:141:THR:HG21	1:A:244:ALA:O	2.17	0.45
1:H:34:ARG:HD3	1:H:61:ALA:O	2.16	0.45
1:D:270:HIS:NE2	2:D:401:HOH:O	2.32	0.45
1:H:129:LYS:HE3	1:H:129:LYS:HB3	1.55	0.45
1:E:254:ARG:HH12	1:H:20:LEU:HA	1.82	0.45
1:B:141:THR:HG21	1:B:244:ALA:O	2.18	0.44
1:D:93:GLN:CD	1:D:285:ARG:HE	2.25	0.44
1:E:20:LEU:O	1:H:254:ARG:HD2	2.18	0.44
1:C:158:ILE:HB	1:C:203:LEU:HD21	2.00	0.44
1:G:100:ASN:ND2	1:G:104:ARG:O	2.34	0.44
1:H:131:ILE:HD11	2:H:408:HOH:O	2.18	0.44
1:H:99:ALA:CB	1:H:278:GLY:HA3	2.43	0.44
1:H:121:PRO:O	1:H:265:ASN:HB3	2.18	0.44
1:F:121:PRO:O	1:F:265:ASN:HB3	2.17	0.44
1:G:121:PRO:O	1:G:265:ASN:HB3	2.18	0.43
1:D:212:ARG:HD3	1:H:280:PHE:CE2	2.53	0.43
1:G:34:ARG:HD3	1:G:61:ALA:O	2.18	0.43
1:E:96:ARG:O	1:E:97:ARG:HB2	2.19	0.43
1:F:20:LEU:O	1:G:254:ARG:HD2	2.19	0.43
1:B:247:PRO:HB3	1:C:139:LEU:HD11	2.01	0.43
1:D:93:GLN:HG3	1:D:285:ARG:HD3	2.01	0.43
1:A:235:PRO:HB2	1:B:235:PRO:HB2	1.99	0.43
1:G:93:GLN:CG	2:G:401:HOH:O	2.65	0.43
1:H:105:VAL:CG1	1:H:274:PRO:HB3	2.48	0.43
1:E:95:ILE:HG13	1:E:126:MET:CE	2.49	0.43
1:E:121:PRO:O	1:E:265:ASN:HB3	2.18	0.43
1:H:72:ARG:HG2	1:H:77:VAL:HG13	2.01	0.42
1:A:82:LEU:HD21	2:A:408:HOH:O	2.20	0.42
1:H:126:MET:HE3	1:H:285:ARG:HB2	2.02	0.42
1:B:121:PRO:O	1:B:265:ASN:HB3	2.19	0.42
1:F:95:ILE:HG13	1:F:126:MET:CE	2.49	0.42
1:G:11:ARG:NE	1:G:11:ARG:HA	2.35	0.42
1:E:248:GLU:HA	1:H:273:VAL:HG13	2.02	0.42
1:F:248:GLU:HG3	1:G:276:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PRO:O	1:A:265:ASN:HB3	2.19	0.42
1:C:121:PRO:O	1:C:265:ASN:HB3	2.19	0.41
1:E:179:ASN:HD22	1:E:179:ASN:N	2.18	0.41
1:G:84:LYS:HB2	1:G:94:MET:HG2	2.02	0.41
1:G:239:PHE:HB2	1:H:235:PRO:HG3	2.01	0.41
1:F:255:TRP:CD1	1:F:281:ARG:HH21	2.39	0.41
1:B:271:TYR:OH	1:C:248:GLU:OE1	2.31	0.41
1:D:121:PRO:O	1:D:265:ASN:HB3	2.20	0.41
1:H:158:ILE:HB	1:H:203:LEU:HD21	2.01	0.41
1:D:246:LYS:O	1:D:247:PRO:C	2.64	0.41
1:H:83:LEU:HD23	1:H:93:GLN:HB3	2.02	0.41
1:G:134:TYR:OH	1:G:279:LYS:HB2	2.21	0.40
1:H:129:LYS:O	1:H:257:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/301 (86%)	246 (95%)	8 (3%)	4 (2%)	7	20
1	B	257/301 (85%)	245 (95%)	7 (3%)	5 (2%)	6	17
1	C	260/301 (86%)	248 (95%)	7 (3%)	5 (2%)	6	17
1	D	259/301 (86%)	246 (95%)	9 (4%)	4 (2%)	8	22
1	E	260/301 (86%)	246 (95%)	9 (4%)	5 (2%)	6	17
1	F	256/301 (85%)	240 (94%)	11 (4%)	5 (2%)	6	16
1	G	271/301 (90%)	254 (94%)	9 (3%)	8 (3%)	3	8
1	H	272/301 (90%)	254 (93%)	12 (4%)	6 (2%)	5	14
All	All	2093/2408 (87%)	1979 (95%)	72 (3%)	42 (2%)	6	16

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	277	ALA
1	B	177	ALA
1	B	277	ALA
1	C	178	GLN
1	C	277	ALA
1	D	178	GLN
1	D	277	ALA
1	E	178	GLN
1	E	277	ALA
1	F	277	ALA
1	G	83	LEU
1	G	84	LYS
1	G	103	GLY
1	G	178	GLN
1	G	179	ASN
1	H	103	GLY
1	H	178	GLN
1	C	276	TYR
1	D	276	TYR
1	F	84	LYS
1	G	82	LEU
1	G	135	GLY
1	H	135	GLY
1	C	82	LEU
1	E	84	LYS
1	F	85	SER
1	H	102	SER
1	B	85	SER
1	B	178	GLN
1	D	85	SER
1	E	85	SER
1	F	276	TYR
1	H	11	ARG
1	A	85	SER
1	C	85	SER
1	G	102	SER
1	H	84	LYS
1	E	135	GLY
1	F	135	GLY
1	A	135	GLY
1	B	135	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/259 (88%)	201 (88%)	26 (12%)	5	14
1	B	226/259 (87%)	203 (90%)	23 (10%)	7	18
1	C	229/259 (88%)	207 (90%)	22 (10%)	8	20
1	D	228/259 (88%)	201 (88%)	27 (12%)	5	13
1	E	228/259 (88%)	203 (89%)	25 (11%)	6	15
1	F	225/259 (87%)	203 (90%)	22 (10%)	7	19
1	G	235/259 (91%)	207 (88%)	28 (12%)	5	13
1	H	236/259 (91%)	209 (89%)	27 (11%)	5	14
All	All	1834/2072 (88%)	1634 (89%)	200 (11%)	6	16

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	31	VAL
1	A	77	VAL
1	A	82	LEU
1	A	83	LEU
1	A	84	LYS
1	A	86	ILE
1	A	96	ARG
1	A	108	GLU
1	A	124	VAL
1	A	125	VAL
1	A	126	MET
1	A	141	THR
1	A	159	GLU
1	A	166	SER
1	A	176	GLN
1	A	178	GLN
1	A	190	MET
1	A	191	ASP

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Mol	Chain	Res	Type
1	A	203	LEU
1	A	217	VAL
1	A	223	GLN
1	A	230	GLU
1	A	236	LEU
1	A	280	PHE
1	A	288	VAL
1	B	18	GLN
1	B	20	LEU
1	B	31	VAL
1	B	77	VAL
1	B	86	ILE
1	B	108	GLU
1	B	118	ASP
1	B	124	VAL
1	B	125	VAL
1	B	126	MET
1	B	130	GLU
1	B	141	THR
1	B	166	SER
1	B	178	GLN
1	B	190	MET
1	B	191	ASP
1	B	203	LEU
1	B	217	VAL
1	B	223	GLN
1	B	230	GLU
1	B	236	LEU
1	B	280	PHE
1	B	288	VAL
1	C	11	ARG
1	C	20	LEU
1	C	31	VAL
1	C	77	VAL
1	C	78	ASP
1	C	84	LYS
1	C	96	ARG
1	C	124	VAL
1	C	125	VAL
1	C	126	MET
1	C	129	LYS
1	C	130	GLU

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Mol	Chain	Res	Type
1	C	141	THR
1	C	166	SER
1	C	178	GLN
1	C	190	MET
1	C	191	ASP
1	C	212	ARG
1	C	217	VAL
1	C	223	GLN
1	C	236	LEU
1	C	288	VAL
1	D	14	ARG
1	D	20	LEU
1	D	31	VAL
1	D	77	VAL
1	D	78	ASP
1	D	82	LEU
1	D	83	LEU
1	D	84	LYS
1	D	93	GLN
1	D	94	MET
1	D	96	ARG
1	D	108	GLU
1	D	124	VAL
1	D	125	VAL
1	D	126	MET
1	D	130	GLU
1	D	141	THR
1	D	166	SER
1	D	178	GLN
1	D	191	ASP
1	D	203	LEU
1	D	212	ARG
1	D	217	VAL
1	D	223	GLN
1	D	236	LEU
1	D	288	VAL
1	D	292	ARG
1	E	20	LEU
1	E	31	VAL
1	E	77	VAL
1	E	82	LEU
1	E	84	LYS

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Mol	Chain	Res	Type
1	E	86	ILE
1	E	96	ARG
1	E	97	ARG
1	E	108	GLU
1	E	124	VAL
1	E	125	VAL
1	E	126	MET
1	E	130	GLU
1	E	141	THR
1	E	166	SER
1	E	178	GLN
1	E	179	ASN
1	E	191	ASP
1	E	203	LEU
1	E	212	ARG
1	E	217	VAL
1	E	223	GLN
1	E	230	GLU
1	E	236	LEU
1	E	288	VAL
1	F	20	LEU
1	F	31	VAL
1	F	77	VAL
1	F	84	LYS
1	F	86	ILE
1	F	96	ARG
1	F	108	GLU
1	F	124	VAL
1	F	125	VAL
1	F	126	MET
1	F	130	GLU
1	F	141	THR
1	F	166	SER
1	F	178	GLN
1	F	212	ARG
1	F	217	VAL
1	F	223	GLN
1	F	230	GLU
1	F	231	LYS
1	F	236	LEU
1	F	276	TYR
1	F	288	VAL

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Mol	Chain	Res	Type
1	G	11	ARG
1	G	13	GLU
1	G	20	LEU
1	G	31	VAL
1	G	77	VAL
1	G	82	LEU
1	G	84	LYS
1	G	86	ILE
1	G	97	ARG
1	G	104	ARG
1	G	105	VAL
1	G	106	ILE
1	G	108	GLU
1	G	124	VAL
1	G	125	VAL
1	G	126	MET
1	G	141	THR
1	G	166	SER
1	G	180	ARG
1	G	203	LEU
1	G	212	ARG
1	G	217	VAL
1	G	223	GLN
1	G	236	LEU
1	G	248	GLU
1	G	254	ARG
1	G	281	ARG
1	G	288	VAL
1	H	10	GLN
1	H	13	GLU
1	H	20	LEU
1	H	31	VAL
1	H	35	GLU
1	H	77	VAL
1	H	82	LEU
1	H	83	LEU
1	H	86	ILE
1	H	104	ARG
1	H	105	VAL
1	H	108	GLU
1	H	124	VAL
1	H	125	VAL

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Mol	Chain	Res	Type
1	H	126	MET
1	H	129	LYS
1	H	141	THR
1	H	166	SER
1	H	212	ARG
1	H	217	VAL
1	H	223	GLN
1	H	236	LEU
1	H	254	ARG
1	H	281	ARG
1	H	285	ARG
1	H	288	VAL
1	H	295	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	179	ASN
1	B	18	GLN
1	B	109	ASN
1	B	178	GLN
1	B	179	ASN
1	D	178	GLN
1	E	178	GLN
1	E	179	ASN
1	G	109	ASN
1	G	178	GLN
1	G	179	ASN
1	H	109	ASN
1	H	178	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	264/301 (87%)	-0.20	0 100 100	48, 62, 115, 139	0
1	B	263/301 (87%)	-0.16	0 100 100	48, 63, 110, 142	0
1	C	266/301 (88%)	-0.06	1 (0%) 88 87	52, 79, 134, 185	0
1	D	265/301 (88%)	-0.10	2 (0%) 82 81	52, 79, 135, 175	0
1	E	266/301 (88%)	-0.33	0 100 100	32, 49, 124, 155	0
1	F	262/301 (87%)	-0.38	0 100 100	31, 50, 112, 161	0
1	G	275/301 (91%)	-0.07	1 (0%) 88 87	43, 77, 122, 157	0
1	H	276/301 (91%)	-0.19	2 (0%) 84 83	42, 77, 120, 159	0
All	All	2137/2408 (88%)	-0.19	6 (0%) 90 89	31, 68, 125, 185	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	282	TYR	2.3
1	D	81	PRO	2.2
1	H	79	PRO	2.1
1	G	48	ALA	2.1
1	D	278	GLY	2.1
1	H	163	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.